AMENDMENTS TO THE CLAIMS

The following listing of claims will replace all prior versions and listings of claims in the application.

LISTING OF CLAIMS

1. (Currently Amended) A three-dimensional quantitative structure-activity relationship method ~~of extracting~~ for determining and visually displaying physiochemical characteristics of a compound ~~based on the atomic coordinates of plural molecules superposed within a virtual space~~ which modulates a pharmacological activity of said compound, the method comprising:

a process A of superposing a three-dimensional spatial arrangement of atoms of a plurality of molecules using Cartesian three-dimensional x, y, and z atomic coordinates in a virtual space;

a process B of performing cluster analysis of the atomic coordinates of said atoms of said plural molecules thus superposed in said virtual space and thereby generating represented points;

a process C of calculating interactions selected from the group consisting of steric interactions, electrostatic interactions, hydrophobic interactions and combinations thereof between the ~~respective~~ atoms of said plural molecules thus superposed and said represented points using an evaluation function; ~~and~~

a process D of statistically analyzing said interactions using statistical analysis to generate a plurality of correlation components between said calculated interactions and a known pharmacological activity of one of said molecules and forming an activity prediction formula[[,]]; and

a process E of assigning an activity prediction value to each atom of said plurality of molecules and displaying said activity prediction value on a graphical display.

wherein said process B of cluster analysis further comprises:

a first process B1 of calculating the coordinates of the ~~respective~~ atoms contained in said plural molecules thus superposed in said virtual space;

a second process B2 of calculating interatomic distances between each atom and other atoms and identifying the shortest interatomic distance among thus calculated interatomic distances and two atoms constituting the shortest interatomic distance;

a third process B3 of deleting said two atoms having the shortest interatomic distance from said three-dimensional space and generating an atom which represents said two atoms in the weighted average coordinates of said two atoms to delete, when the shortest interatomic distance thus calculated is equal to or smaller than a predetermined threshold value;

a fourth process B4 of returning to said second process B2 after said third process B3 and executing said second process B2 including said atoms formed during said third process B3; and

a fifth process B5 of terminating said process B when the shortest interatomic distance thus calculated is exceeds said predetermined threshold.

2. (Cancelled)

3. (Cancelled)

4. (Currently Amended) A program for a three-dimensional quantitative structure-activity relationship method ~~of extracting~~ for determining and visually displaying physicochemical characteristics of a compound which ~~based on the atomic coordinates of plural molecules superposed within a virtual space~~ which modulates a pharmacological activity of said compound, said program making a computer execute:

a process A of superposing a three-dimensional spatial arrangement of atoms of a plurality of molecules using Cartesian three-dimensional x, y, and z atomic coordinates in a virtual space;

a process B of performing cluster analysis of the atomic coordinates of said plural molecules thus superposed in said virtual space and thereby generating represented points;

a process C of calculating interactions selected from the group consisting of steric interactions, electrostatic interactions, hydrophobic interactions and combinations thereof between the ~~respective~~ atoms of said plural molecules thus superposed and said represented points using an evaluation function; ~~and~~

a process D of statistically analyzing said interactions using statistical analysis to generate a plurality of correlation components between said calculated interactions and a known pharmacological activity of one of said molecules and forming an activity prediction formula[[,]]; and

a process E of assigning an activity prediction value to each atom of said plurality of molecules and displaying said activity prediction value on a graphical display.

wherein said process B of cluster analysis further comprises:

a first process B1 of calculating the coordinates of the ~~respective~~ atoms contained in said plural molecules thus superposed in said virtual space;

a second process B2 of calculating interatomic distances between each atom and other atoms and identifying the shortest interatomic distance among thus calculated interatomic distances and two atoms constituting the shortest interatomic distance;

a third process B3 of deleting said two atoms having the shortest interatomic distance from said three-dimensional space and generating an atom which represents said two atoms in the weighted average coordinates of said two atoms to delete, when the shortest interatomic distance thus calculated is equal to or smaller than a predetermined threshold value;

a fourth process B4 of returning to said second process B2 after said third process B3 and executing said second process B2 including said atoms formed during said third process B3; and

a fifth process B5 of terminating said process B when the shortest interatomic distance thus calculated is exceeds said predetermined threshold.

5. (Cancelled)

6. (Cancelled)

7. (New) The method according to Claim 1, wherein the process C of calculating interactions includes an evaluation formula selected from the group consisting of rapid molecular superstition, seal-type, indicated variables and combinations thereof.

8. (New) The method according to Claim 4, wherein the process C of calculating interactions includes an evaluation formula selected from the group consisting of rapid molecular superstition, seal-type, indicated variables and combinations thereof.